

NAGW-766

7N-72-UR

59 252407

128

# ATOMIC DATA BASE AND THE U.K.-U.S. OPACITY PROJECT

A. K. Pradhan  
 Joint Institute for Laboratory Astrophysics  
 University of Colorado and National Bureau of Standards  
 Boulder, CO 80309-0440

## ABSTRACT

With the primary aim of calculating stellar envelope opacities, a joint international collaboration is under way for the calculation of basic atomic data for radiative processes: oscillator strengths, photoionization cross sections, energy levels, radiative damping constants (including line broadening). Atomic calculations have been completed for the first ten isoelectronic sequences, H-like to Ne-like, going up to iron, and work is in progress on the third and fourth row atoms and isosequences. The close-coupling approximation is employed throughout using a new version of the R-matrix method. Particular emphasis is placed on the detailed resolution of autoionization structures in the bound-free continuum.

## I. INTRODUCTION

A general description of the Opacity Project is given in the first of a series of papers entitled "Atomic Data for Opacity Calculations" or ADOC I-VII<sup>1</sup> and in Ref. 2.

Elementary radiative processes involving light absorption and scattering determine the opacities in the envelope region of stellar atmospheres characterized by the general range of plasma parameters given in Table 1. An accurate calculation of these opacities is rendered difficult by the vast amount of requisite atomic data for the bound-bound and the bound-free radiative processes, and associated plasma effects, in essentially all the atoms and ions normally abundant. Furthermore, the final results depend upon the accuracy of the atomic data input incorporating the important atomic effects, such as autoionization structures that are known to be present extensively in the bound-free continuum. In addition, plasma effects such as line broadening and the pressure broadening of autoionization

Table 1. Typical plasma parameters in stellar envelopes

Log T	Log $\rho$	Log P	Log $N_e$
(K)	(g cm <sup>-3</sup> )	(dynes)	(cm <sup>-3</sup> )
4.5	-8.5	3.9	15.3
5.0	-7.0	5.9	16.8
5.5	-5.0	8.0	18.3
6.0	-3.5	10.3	20.3
6.5	-1.5	12.9	22.3

© American Institute of Physics 1988

(NASA-CR-186145) ATOMIC DATA BASE AND THE  
 U.K.-US OPACITY PROJECT (Joint Inst. for  
 Lab. Astrophysics) 12 p

N90-70391

Unclas  
 00/72 0252407

resonances must be properly accounted for. The present Opacity Project involves new approaches to these problems and also includes a new equation-of-state method,<sup>3-5</sup> based on free-energy minimization, for the calculation of internal atomic partition functions that provide the occupation probabilities for level populations.

The basic theoretical methods, and related computational techniques, for the atomic physics calculations were developed during the past two decades. Particularly from the mid-70's onward a significant number of accurate calculations for the radiative and collisional processes have been carried out employing large computational packages based on the close-coupling approximation of atomic collisions theory. The total number of these calculations was still rather small since they required an enormous investment of manpower and computing resources. However, recent theoretical and computational breakthroughs under the auspices of the Opacity Project, coupled with the availability of supercomputers, now enable us to carry out systematic and accurate calculations on a large scale for most of the atoms and ions of interest in astrophysical and laboratory plasmas. The R-matrix method, described in Sec. III, provides the most efficient means for atomic calculations, in the close-coupling approximation, and is employed for nearly all of the present work.

In previous works on envelope opacities,<sup>6-8</sup> much simpler atomic models have been used and it appears that they may have underestimated the metal opacities by a factor of 2 or 3, as evidenced by the problems encountered in theories and observations of stellar pulsation and evolution.<sup>9,10</sup> Although it is too early to conclude whether the new opacity calculations would account for these discrepancies, it is worthwhile to employ the most accurate state-of-the-art atomic physics to recalculate, *ab initio*, all the basic atomic data contributing to the opacities.

The main scope of the present Opacity Project is the computation of the oscillator strengths and photoionization cross sections involving the first ten isoelectronic sequences, H to Ne, up to and including iron; atoms and ions with  $Z = 1-14, 16, 18, 20$  and  $26$  are considered explicitly. In addition, all ions of iron and of the cosmically abundant elements with  $14 < Z < 26$  are also included. The R-matrix calculations entail all bound states of each atom or ion with  $n \leq 10$  and  $l \leq 3$  i.e. all resulting multiplets characterized by a total spin and angular momenta,  $SL$ . It is estimated that one would obtain approximately 200-500 bound states per ion or atom and a total of  $10^6 - 10^7$  oscillator strengths. Photoionization cross sections for all the levels will be tabulated at approximately 1000 - 2000 energies per level (in order to take account of the detailed resonance structures).

The atomic data produced through these calculations is analyzed and retabulated at a mesh of photon frequencies to obtain the opacities (incorporating the equation-of-state parameters). The highly accurate atomic data base thus created is also expected to be useful in a wide variety of laboratory and astrophysical plasmas.

## II. RADIATIVE PARAMETERS

The radiated flux propagating through a stellar envelope is governed by the Rosseland mean opacity defined in terms of the inverse of the absorption coefficient as

$$\frac{1}{\kappa_R} = \int_0^\infty \frac{1}{k_\nu} g(u) du, \quad (2.1)$$

where  $k_\nu$  is the monochromatic opacity coefficient,  $u = h\nu/kT$ , and  $g(u)$  is a weighting function incorporating the black-body distribution with a correction for stimulated emission and is given by

$$g(u) = \left(\frac{15}{4\pi}\right) u^4 \exp(-u) [1 - \exp(-u)]^{-3}. \quad (2.2)$$

The total monochromatic opacity  $k_\nu$  is the sum over all contributing radiative processes, in particular the bound-bound and the bound-free absorption. Corresponding to line absorption and photoionization from a bound state  $i$ , we have

$$k_\nu(i) = N(X_i) \sigma_\nu(i) \phi_p(\nu) \quad (2.3a)$$

and

$$k_\nu(i \rightarrow j) = N(X_i) \frac{2\pi^2 e^2}{mc} f_{ij} \phi_e(\nu), \quad (2.3b)$$

where  $N(X_i)$  is the level population and  $\sigma_\nu(i)$  and  $f_{ij}$  are the photoionization cross section and the oscillator strength respectively. In (2.3a,b) we have also included the profile factors,  $\phi_p(\nu)$  and  $\phi_e(\nu)$ , due to electron pressure and plasma microfield broadening of autoionization and line features. In particular the collisional broadening damping constants may be defined by writing the appropriate line profile factor as

$$\phi_e(\nu) = \frac{\gamma/2\pi}{(\nu + \frac{1}{2}\epsilon - \nu_0)^2 + (\frac{1}{2}\gamma)^2}, \quad (2.4)$$

where the width  $\gamma$  and the shift  $\epsilon$ , from line center  $\nu_0$ , are proportional to electron density i.e.

$$\gamma + i\epsilon = Ne\Gamma, \quad (2.5)$$

with  $\Gamma$  as the collisional damping constant which is a complex quantity. Following Baranger,<sup>11</sup> one may express  $\Gamma$  in the impact approximation in terms of thermally averaged collision strengths for electron-ion scattering. The appropriate scattering matrices for the initial and the final states may be obtained accurately from the atomic collision methods employed in the present work for a number of low lying transitions in the ions considered. A Bethe-type approximation has been developed, applicable to all other transitions, which yields a general expression for  $\Gamma$  in terms of a slowly varying  $z$  (ion charge) dependent factor and radiative transition probabilities for all transitions from the initial and the final states.<sup>12</sup> The latter

approximation agrees closely, well within 50% for most cases, with the quantum mechanical calculations for the low lying transitions.

In addition to collisional broadening, one also needs to account for the Doppler width at local temperatures and the Stark effect due to plasma micro-fields. For non-hydrogenic systems one expects the collisional broadening effect to be the dominant effect, subsuming the Doppler width as well as the fine structure separations. However, for hydrogenic systems the Stark effect is expected to make a large contribution and work is in progress to develop methods similar to those for collisional broadening mentioned above. It is also expected that the broadening of autoionization features in the photoionization cross sections can be treated on the same basis as line broadening, with simple expressions to convolute the detailed cross sections. It appears rather important to address this problem since the form of the Rosseland opacity (2.1) indicates that the minima in  $k_\nu$ , associated with resonances in the bound-free cross sections, would make a significant contribution to the integral and therefore the structure of these "holes" in the opacities needs to be considered carefully.

### III. ATOMIC CALCULATIONS

The computational methods are described in ADOC I<sup>1</sup> and subsequent publications. Briefly, the basic method is the close-coupling approximation of atomic collision theory that enables an accurate computation of electron + atom (ion) system with the electron at either positive or negative energies. Thus, both the continuum and the bound state atomic wavefunctions can be obtained. A variety of collisional and radiative parameters can be calculated thereby: scattering and photoionization cross sections, transition probabilities, etc. The close-coupling approximation involves the solution of coupled integro-differential equations, which can be solved in the most efficient manner with the R-matrix method developed by Burke and co-workers. An outline of the close-coupling approximation and the R-matrix method is as follows.

The total e + atom wavefunction may be written as an expansion in terms of products of atomic eigenfunctions and the wavefunction of the free electron:

$$\psi^{SL\pi} = \sum_i (\psi_i \theta_i) SL\pi + \sum_j c_j \phi_j^{SL\pi} \quad (3.1)$$

where  $SL\pi$  is the total spin, angular momentum and parity of the e + atom system;  $\psi_i$  are the atomic eigenstates,  $\theta_i$  is the free electron function and  $\phi_j$  are e + atom bound state wavefunctions included to satisfy orthogonality constraints and additional short range correlation effects. The  $\theta_i$  and the coefficients  $c_j$  are treated as variational parameters in the close-coupling approximation and variation with respect to these quantities yields a set of coupled integro-differential equations which account for the coupling between the atomic eigenstates included in the first term of (3.1). The number of such states, usually referred to as "target" (or "parent" or "core") states, generally comprises the terms dominated by the lowest few

electronic configurations of the atom (target) under consideration. Implicit in the summation in the first term of (3.1) is the sum over the orbital angular momenta " $l$ " of the free electron; these are usually fairly low " $l$ " values (simpler approximations may be used for higher  $l$ 's). For radiative problems, it is evident that bound states of the  $e + \text{atom}$  system may be treated hydrogenically if  $l > 3$ , since the quantum defect is nearly zero and the resulting state is hydrogen-like. Thus in the present work detailed R-matrix calculations are generally carried out for the atomic target states coupled with  $l \leq 3$ .

The R-matrix method consists of dividing up the configuration space into an inner and an outer region. In the inner region one takes into account the short range interactions between all the electrons of the total electron + atom system, in particular the exchange effect due to antisymmetrization represented by the operator  $\Lambda$  in (3.1). Solutions in the outer region are simpler as they include only the long range interactions between the electron and the atom (for example, exchange is neglected). The boundary between the inner and the outer regions, is taken to be such that the atomic eigenfunctions are negligibly small. The inner region solutions of  $\Psi(e + \text{atom})$  are expanded in terms of a basis set of functions that satisfy the R-matrix boundary conditions at, say,  $r = a$ , i.e.,

$$\left. \frac{\frac{d}{dr} f_l(r)}{f_l(r)} \right|_{r=a} = b, \quad (3.2)$$

the  $\{f_l(r)\}$  are the radial part of the set  $\{\psi_n\}$  in terms of which the total wavefunction (3.1) is expanded at any energy  $E$ , i.e.,

$$\Psi_E = \sum_n \psi_n A_{nE}. \quad (3.3)$$

The coefficients  $A_{nE}$  are obtained on diagonalization of the Hamiltonian of the  $e + \text{atom}$  system and are given as

$$A_{nE} = \frac{\sum_l f_{ln}(r) \left. \frac{d}{dr} F_l(r) \right|_{r=a}}{(e_n - E)}, \quad (3.4)$$

where the  $e_n$  are the eigenvalues of the R-matrix basis functions  $\{\psi_n\}$ ; the  $F_l(r)$  represents the radial part of  $\Psi_E$  in (3.1) and is given in terms of the R-matrix as

$$F_l(r) = \sum_1 R_{11,}(E) \left. \frac{d}{dr} F_1(r) \right|_{r=a}, \quad (3.5)$$

where

$$R_{11,}(E) = \frac{\sum_n f_{1n}(a) f_{1,n}(a)}{(e_n - E)}. \quad (3.6)$$

An especially useful feature of the R-matrix method is that once the R-matrix basis functions are determined by diagonalization of the  $e +$  atom Hamiltonian for each symmetry  $SL$ , the full solutions  $\psi_E^{SL}$  may be obtained readily at any energy, thus enabling a rapid computation of cross sections and transition probabilities, etc., corresponding to a large number of energies. This is especially important when the cross sections contain extensive resonance structures. For example, in the present work it is found that the photoionization cross sections need to be calculated at 1000 - 2000 energies for each bound state. As mentioned earlier, the detailed resonance features may be crucially important in the final opacities, in particular the Rosseland mean.

For bound-bound transitions, we calculate the dipole matrix elements in the inner region I in terms of the R-matrix basis functions as

$$D_I(n, n') = (\psi_n | D | \psi_{n'}) \quad (3.7)$$

The dipole matrix element with the wavefunctions for the "physical" bound states  $\psi_E$  and  $\psi_{E'}$  ( $E, E' < 0$ ) is then given by

$$D_I(E, E') = \sum_{n, n'} A_{nE}^* D_I(n, n') A_{n'E'} \quad (3.8)$$

The total dipole matrix element for the transition between the bound states of the  $e +$  atom system at energies  $E$  and  $E'$  is obtained on adding to (3.8) the contribution from the outer region, employing solutions of  $\psi_E$  and  $\psi_{E'}$  neglecting short range interactions. For the bound-free transitions we calculate the dipole matrix elements with wavefunctions for a bound state with  $E < 0$  and a continuum state with  $E > 0$ .

It is convenient to carry out the atomic calculations along isoelectronic sequences since the target electronic configurations are the same for all ions in the sequence. However, the correlation effects may be different for low  $Z$  ions as opposed to high  $Z$  ones and therefore different configuration interaction bases may be used to represent the eigenfunction expansions for ions in a sequence, depending upon the nuclear charge. The variational principle employed in the derivation of the close-coupling equations is based on the assumption that the target atomic eigenfunctions are known exactly. It is therefore imperative to obtain an accurate representation for the eigenstates included in (3.1). We employ two independent atomic structure programs to calculate configuration interaction type wavefunctions for the target eigenstates: the program CIV 3 by Hibbert<sup>13</sup> using Clementi-type Hartree-Fock orbitals optimized to obtain the individual target state functions, and the program SUPERSTRUCTURE by Eissner et al.<sup>14</sup> using a scaled Thomas-Fermi-Dirac potential to generate the one-electron orbitals, and thereby the wavefunctions for all the eigenstates included in the close-coupling expansion. Both programs yield results of comparable accuracy when optimized properly. The atomic structure programs provide output in terms of angular and radial parameters which are input to the main R-matrix package which consists of several programs, designated by the prefix

STG, corresponding to the various stages of the calculations, e.g., STGR for radial integrals (formerly STG1), STGA for angular algebra (formerly STG2), STGH for the diagonalization of the  $e + \text{atom}$  Hamiltonian (formerly part of STG3), STGB for the calculation of bound state wavefunctions, STGF for the continuum wavefunctions (also collision strengths), STGBB for bound-bound data (oscillator strengths), STGBF for the bound-free (photoionization cross sections) and STGD for collisional damping constants for line broadening.

#### IV. INTERFACE BETWEEN ATOMIC DATA AND OPACITY CALCULATIONS

The rather huge amount of atomic data required for the opacity calculations needs to be analyzed, processed and mapped onto a frequency grid in incident photon frequencies. The "interface" stage involves the interpolation of the atomic data, originally tabulated relative to atomic eigenenergies, into a pre-determined frequency mesh. Corresponding to the atomic and ionic species abundant in the range of parameters given in Table 1, we have chosen  $\log_{10} T_{\min} = 3$  and  $\log_{10} T_{\max} = 7$  and photon frequencies  $\log_{10} \nu_{\min} = 10.6188$  and  $\log_{10} \nu_{\max} = 18.6188$ . The frequency interval is chosen to be  $\Delta \log_{10} \nu = 3.90625 \times 10^{-6}$ . The precise values of frequencies are determined for computational convenience.

As we are dealing with a large number of excited states of each atom or ion, typically 300, it is necessary to determine the spectroscopic identity of all the bound states. Although this requirement is not essential to the opacity calculations, it is useful in the analysis and tabulation of atomic data and, perhaps more importantly, should enable the diagnostics of opacities over specific regions in terms of the underlying atomic physics. In addition, most of the atomic data are being calculated for the first time and the data base should have wide ranging applications in other areas such as fusion, laser technology, optical and chemical physics, etc. The level identification of some excited states can be problematic due to configuration mixing in cases where no one configuration makes the dominant contribution to the given state. However, we have developed algorithms for fairly precise determination of spectroscopic designation. We might note here that the number of atomic bound states calculated under the Opacity Project far exceeds the number that are observationally determined and, given the accuracy of the present calculations, should be a useful contribution to atomic spectroscopy.

The bound-bound oscillator strengths are tabulated at frequencies corresponding to the closest indices on the opacity mesh, whereas the bound-free photoionization cross sections, originally given as a function of the continuum electron energy, are interpolated to the closest mesh indices over the range of photoionization from threshold up to frequencies where the cross section has decreased to very small values. Parameters for radiative damping and collisional broadening are also given.

The analysis and interface of atomic data are carried out by the program INTFACE, which produces the bound-bound and the bound-free data files for the program OPACITY, which calculates the opacities in

segments of the frequency grid. The calculations are carried out on the Cray-XMP at the National Center for Supercomputer Applications in Urbana, Illinois. The atomic data files are to be stored on the SSD (solid-state-device for storage of large data files), and are input to the opacity program according to the mesh segment (or "window") under consideration, i.e., the OPACITY program determines and calls in only the data files for the atoms and ions corresponding to the absorption frequencies within the segment.

## V. SAMPLE RESULTS

In this section we describe briefly the calculations and the results for one atom, neutral carbon, which might serve to exemplify the typical aspects of the atomic physics involved. In the close-coupling approximation the C I radiative calculations begin with the "target" or the "parent" ion C II. From the expansion (3.1) we include the first term eigenstates of C II that are dominated by the configurations:  $1s^2 2s^2 2p$  ( $2p^0$ ),  $1s^2 2s 2p^2$  ( $4p, 2D, 2S, 2p$ ),  $1s^2 2s^2 3s$  ( $2S$ ),  $1s^2 2s 2p^2$  ( $2p^0$ ) and  $1s^2 2p^3$  ( $4s^0, 2p^0, p^0$ ). The eigenfunction representation of these states includes electronic correlation from the following configurations:  $1s^2 2s^2 3d$ ,  $2s 2p^3 s$ ,  $2s^2 4s$ ,  $2s^2 4p$ ,  $2s^2 4d$ ,  $2s 2p^3 p$ ,  $2s 2p^3 d$ ,  $2p^2 3s$ ,  $2p^2 3p$ ,  $2s 3p^3 d$ ,  $2s 3d^2$ ,  $2s 3s^3 p$ ,  $2p^2 3d$ ,  $2p^2 4s$ ,  $2p^2 4p$ ,  $2s 3s^2$ ,  $2s 3p^2$ ,  $2p^3 s^3 p$  and  $2p^3 s^3 d$ . Thus a 23 configuration expansion is used to represent the core states accurately. The close-coupling approximation then involves the solution of the coupled integro-differential equations for the  $(e + \text{CII})$  system using the R-matrix method, in several stages, as described earlier. The orbital angular momenta of the additional electron are taken to be  $l \leq 3$  (i.e. s, p, d, f). We obtain all C I bound states of the type  $(\text{C II}, S_1 L_1) n l$  with  $n \leq 10$ ,  $l \leq 3$ . For example, a typical series of states would be  $[2s^2 2p$  ( $2p^0$ )]  $3s, \dots, 10s$ , up to  $[4f, \dots, 10f$  (in addition to the equivalent electron states belonging to C I configurations such as  $2s^2 2p^2$ ,  $2s 2p^3$  etc.).

Figure 1 illustrates the photoionization cross sections for the three states of C I dominated by the ground configuration  $2s^2 2p^2$  ( $3P, 1D, 1S$ ). The ten ionization thresholds corresponding to the eigenstates of C II are indicated. Several Rydberg series of resonances are seen to converge onto the excited thresholds. For the ground state,  $3P$ , the cross sections are in good agreement ( $< 5\%$ ) with the earlier R-matrix calculations by Taylor and Burke<sup>15</sup> and the detailed resonance structure follows closely both the earlier theoretical results as well as the experimental cross sections measured by Esteve et al.<sup>16</sup>

A total of 4763 oscillator strengths were calculated for neutral carbon. In Table 2 we compare a few selected oscillator strengths with those calculated by Nussbaumer and Storey<sup>17</sup> (NS) who also employed the close-coupling approximation. The present results are labeled OP (for Opacity Project) and are given in both the length (L) and the velocity (V) formulations. With the exception of weak transitions, the agreement between the three sets of data is well within 10%. Figure 2 illustrates the agreement between the L and V oscillator strengths for all transitions with  $f_L, f_V \geq 0.01$ . It is seen that



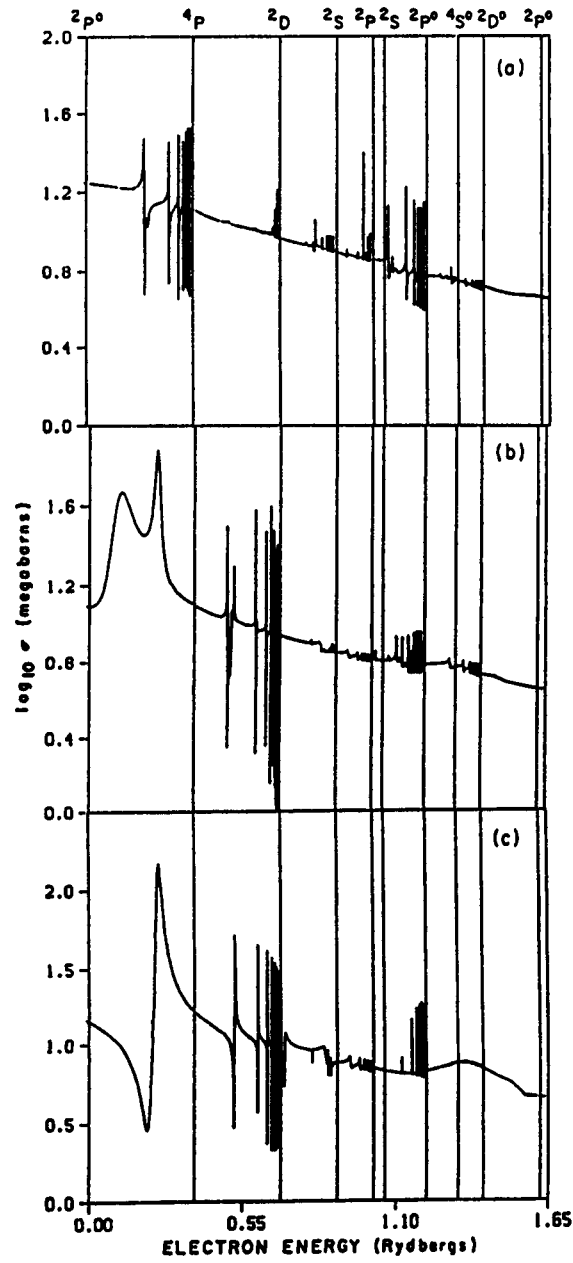


Fig. 1. Photoionization cross sections of ground configuration states of neutral carbon: (a)  $\sigma(^3P)$ , (b)  $\sigma(^1D)$ , (c)  $\sigma(^1S)$ . The C II ionization thresholds are shown by vertical lines.

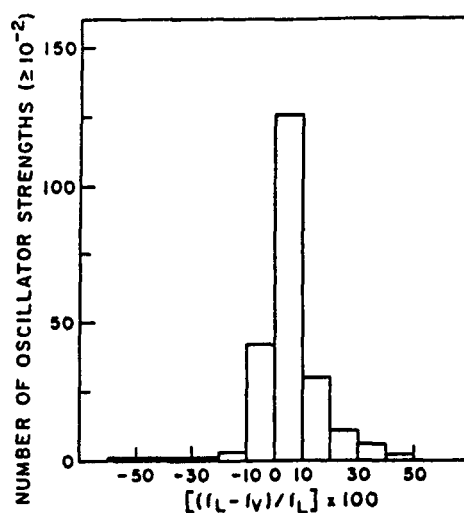


Fig. 2. Percentage-wise agreement between length and velocity oscillator strengths of C I (for all transitions with  $f_L, f_V \geq 0.01$ ).

Table 2. Oscillator Strengths for C I

Transition	$\lambda(\text{\AA})$	$f_L^{\text{OP}}$	$f_V^{\text{OP}}$	$f_L^{\text{NS}}$
$2s^2 2p^2 (3P) - 2s^2 2p 3s (3P^o)$	1657.2	1.476(-1)	1.497(-1)	1.394(-1)
$(3P) - 2s^2 2p^3 (3D^o)$	1561.1	6.95 (-2)	7.35 (-2)	6.973(-2)
$(3P) - 2s^2 2p 3d (3D^o)$	1277.5	1.094(-1)	1.064(-1)	9.407(-2)
$(1D) - 2s^2 2p^3 s (1P^o)$	1930.9	1.202(-1)	1.167(-1)	1.138(-1)
$(1S) - 2s^2 2p 3s (1P^o)$	2478.6	8.53 (-2)	8.38 (-2)	8.620(-2)
$2s^2 2p 3s (3P^o) - 2s^2 2p 3p (3D)$	10693.4	4.933(-1)	5.440(-1)	5.073(-1)
$(3P^o) - (3S)$	9639.7	1.062(-1)	1.104(-1)	1.070(-1)
$2s^2 2p^3 (3D^o) - 2s^2 2p 3p (3D)$	17747.2	1.800(-3)	3.200(-3)	1.854(-3)
$2s^2 2p 3p (1P) - 2s^2 2p 3d (1D^o)$	11330.3	6.937(-1)	5.573(-1)	6.706(-1)
$(3D) - 2s^2 2p^3 (3P^o)$	18068.7	1.310(-2)	1.420(-2)	1.046(-2)
$(3P) - 2s^2 2p 4s (3P^o)$	14793.3	5.290(-2)	7.210(-2)	3.348(-2)

for most of the 275 transitions considered, the agreement is within  $\pm 10\%$ .

## VI. EXTENSION TO COLLISIONAL DATA

The calculation of LTE opacities requires mainly the data for radiative processes (with some computations for collisional broadening). The same basic theoretical and computational methods may be employed for electron-ion collisions. However, the radiative and collisional calculations are, in general, not carried out in the same manner. For collisional excitation it may be necessary to use a much larger eigenfunction expansion in terms of the target atomic states [Eq. (3.1)] in order to obtain cross sections involving a number of target states; whereas the contribution to opacities from states belonging to excited parent configurations is usually small. For example, in the present work it is considered sufficient to include only the ground state of ions in the helium and neon isoelectronic sequences to obtain the radiative data for Li-like ( $e + \text{He-like}$ ) and Na-like ( $e + \text{Ne-like}$ ) atoms and ions respectively. However, for electron impact excitation, a number of excited states (approximately 10 or greater) are of practical interest. A second difference lies in the number of partial waves of the additional electron; again, for collisional calculations one may need to include a larger number of partial waves than for radiative calculations since in the radiative case bound states with  $l \geq 3$  are hydrogen-like and need not be calculated by the close-coupling method but may be readily obtained in the hydrogenic approximation.

A logical extension of the Opacity Project would be to consider the various collisional processes within the same framework. At present, collision strengths may also be calculated, in the LS approximation, employing the new computational package. Work is in progress to include the fine structure in the atomic target states and to extend the calculations to dielectronic recombination cross sections.

## VII. ATOMIC DATA BASE

The unprecedented magnitude and accuracy of the atomic data produced under the auspices of the Opacity Project should be useful for many applications involving the analysis of laboratory and astrophysical plasmas. Procedures may be developed to identify and process the data in accordance with the intended application. It is planned to establish the data bases at the Daresbury Laboratory in the U. K. managed by the U. K. members of the Project, and at the NCSA in Urbana by the U. S. members of the team. The bulk of the data will consist of: energy levels, oscillator strengths, photoionization cross sections, radiative and collisional damping constants and recombination coefficients. To date, calculations have been completed for the first ten isoelectronic sequences, from H-like to Ne-like. Approximately  $10^6$  oscillator strengths have been obtained along with photoionization cross sections for 200-400 bound states in each ion, tabulated at a fine energy mesh. Work is in progress on several isosequences in the third row of the periodic table, as well as on all iron ions.

## ACKNOWLEDGMENTS

The Opacity Project team is led by M. J. Seaton at University College London. D. Mihalas and D. G. Hummer are responsible for developing the equation-of-state code for envelope opacities. The effort at the Queen's University of Belfast is led by P. G. Burke. The atomic calculations are being carried out at Belfast, Boulder, Caracas, London, Meudon, and Munich; the researchers involved are K. A. Berrington, V. M. Burke, K. Butler, W. Eissner, J. A. Fernley, A. Hibbert, A. E. Kingston, D. J. Lennon, D. Luo, A. K. Pradhan, H. E. Saraph, P. J. Storey, K. T. Taylor, J. Tully, and C. Zeippen.

The author would like to thank D. Luo for assistance with the calculations reported here. This contribution was supported by a NASA grant (NAGW-766).

## REFERENCES

1. M. J. Seaton, ADOC I, J. Phys. B. 20, 6363 (1987).
2. A. K. Pradhan, Physica Scripta 35, 840 (1987).
3. D. G. Hummer and D. Mihalas, Astrophys. J. (in press).
4. D. Mihalas, W. Dappen and D. G. Hummer, Astrophys. J. (in press).
5. W. Dappen, D. Mihalas, D. G. Hummer and B. W. Mihalas, Astrophys. J. (in press).
6. A. N. Cox, in Stars and Stellar Systems ed. L. H. Aller and D. B. Laughlin (Chicago University Press, 1965), p. 195.
7. T. R. Carson, Ann. Rev. Astron. Astrophys. 130, 279 (1984).
8. W. F. Huebner, in Physics of the Sun ed. P. Sturrock, T. Holzer, D. Mihalas and R. Ulrich (Dordrecht: Reidel, 1985), p. 33.
9. N. R. Simon, Astrophys. J. 260, L87 (1982); in Stellar Pulsation, ed. A. N. Cox, W. M. Sparks and S. G. Starrfield (Springer-Verlag, 1986), p. 148.
10. G. Bertelli, A. G. Bressan and C. Chiori, Astron. Astrophys. 130, 279 (1984).
11. M. Baranger, Phys. Rev. 111, 494 and 112, 855 (1958).
12. M. J. Seaton, J. Phys. B. (submitted).
13. A. Hibbert, Comput. Phys. Commun. 9, 141 (1975).
14. W. Eissner, M. Jones and H. Nussbaumer, Comput. Phys. Commun. 8, 270 (1974).
15. K. T. Taylor and P. G. Burke, J. Phys. B 9, L353 (1976).
16. J. M. Esteva, G. Mehlmann-Balloffit, and J. Romand, J. Quant. Spec. Rad. Transf. 12, 1291 (1972).
17. H. Nussbaumer and P. J. Storey, Astron. Astrophys. 140, 383 (1984).